Sandia National Laboratories, California
Thin-Film & Interface Research Program

Highlights 1998

Science of Metals

Advanced Ceramics

Alloy Theory

Interfacial Dislocation Dynamics

Observation and Modeling of the Core Structure of Dissociated $\frac{1}{3} < 111 >$ Twin Dislocations

D.L. Medlin and S.M. Foiles

Motivation:

The dynamic behavior of interfaces is controlled in part by the properties of interfacial defects. In recent work we have discovered a mechanism by which *climb* of $\frac{1}{3} < 111 >$ interfacial dislocations can lead to twin growth in FCC materials [D.L. Medlin *et al.*, Phil. Mag. A 75 (3) (1997) 733-747]. This mechanism is quite distinct from conventional twinning, which occurs by *glide* of 1/6<112> dislocations. Until now, however, the core structure of these interfacial dislocations has been poorly understood.

Accomplishment:

We have combined atomistic modeling and HRTEM imaging to determine the core structure for a $\frac{1}{3} < 111 >$ twin dislocation in aluminum. Figure 1 shows the atomic positions for this defect as predicted using the Embedded Atom Method (Ercolessi-Adams Al potential). In Figure 2 the intensity peak positions from an HRTEM image simulation for the calculated structure are overlaid on the experimentally observed lattice image of a $\frac{1}{3} < 111 >$ twin dislocation. Both the calculation and observation show that the dislocation is in a dissociated configuration. As indicated by the dashed lines on Figures 1 and 2, the center of the dislocation core is positioned away from the coherent twin interface by a distance of about three {111} planes. This atomic configuration can be understood in terms of a classical dislocation dissociation reaction. As is illustrated in Figure 3, the perfect $\frac{1}{3}[\bar{1}\,\bar{1}\,\bar{1}]$ twin dislocation ($\delta\mathbf{D}$ in Thompson's notation) may dissociate by emitting from the interface a Shockley partial dislocation ($\mathbf{b}=\frac{1}{6}[\bar{2}\,\bar{1}\,\bar{1}] = \beta\mathbf{D}$) onto the $(1\,\bar{1}\,\bar{1})$ plane (which is inclined with respect to the (111) twinning plane). This produces a short segment of stacking fault on the $(1\,\bar{1}\,\bar{1})$ plane and leaves behind a stair-rod dislocation ($\mathbf{b} = \frac{1}{6}[0\,\bar{1}\,\bar{1}] = \delta\beta$) at the twin step.

Significance:

Our observations that the $\frac{1}{3} < 111 >$ twin dislocation possesses an extended dislocation core refines our earlier model for twin growth by dislocation climb, which treated the dislocation core as compact. The result poses a critical question: must the defect constrict to a compact configuration before absorbing a vacancy and climbing or can the absorption occur along the extended defect? We are currently calculating the energetics of the possible vacancy configurations at the dissociated interfacial dislocation in order to resolve this issue. Ultimately, this work will help to provide an atomic scale basis for understanding interfacial motion induced by dislocation climb.

Publications:

Observation and Modeling of $\frac{1}{3} < 111 >$ Twin Dislocations in Aluminum, D.L. Medlin, to be published in: Advances in Twinning. eds. S. Ankem and C.S. Pande (TMS, 1999).
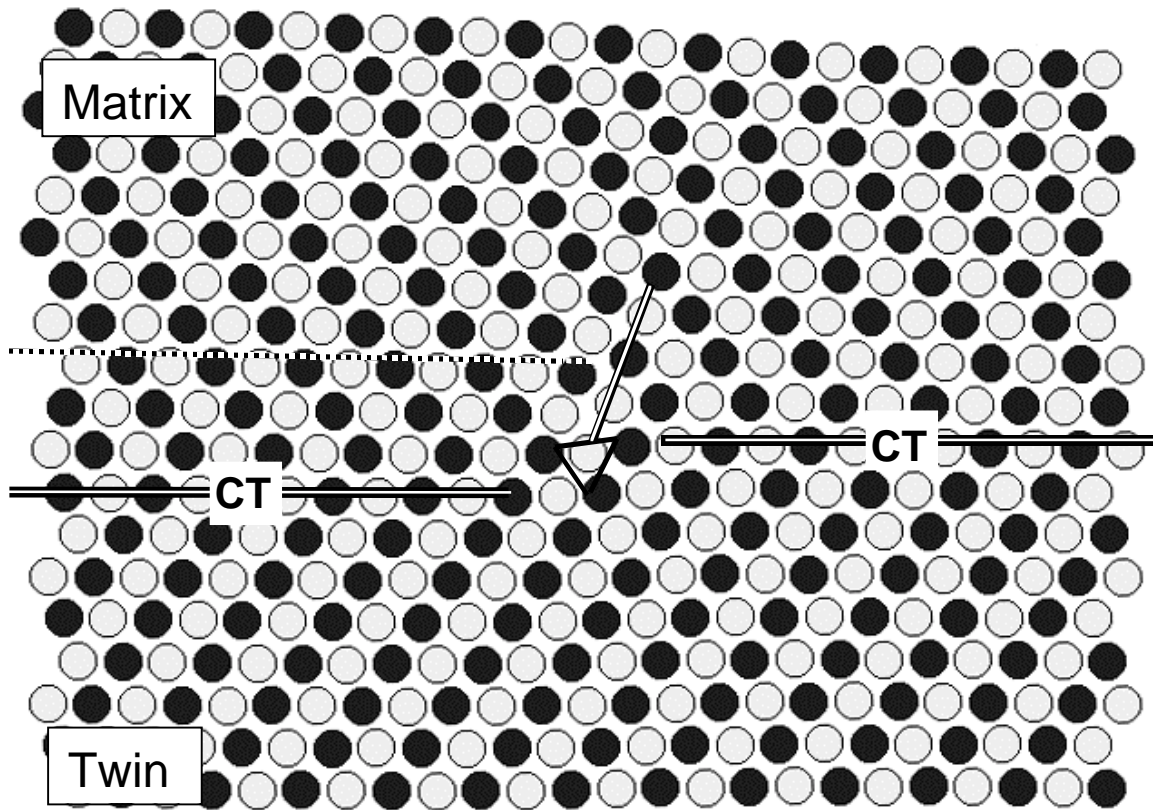
Figure 1: Relaxed structure for $\frac{1}{3}[\bar{1}\,\bar{1}\,\bar{1}]$ interfacial dislocation at twin interface in Aluminum.

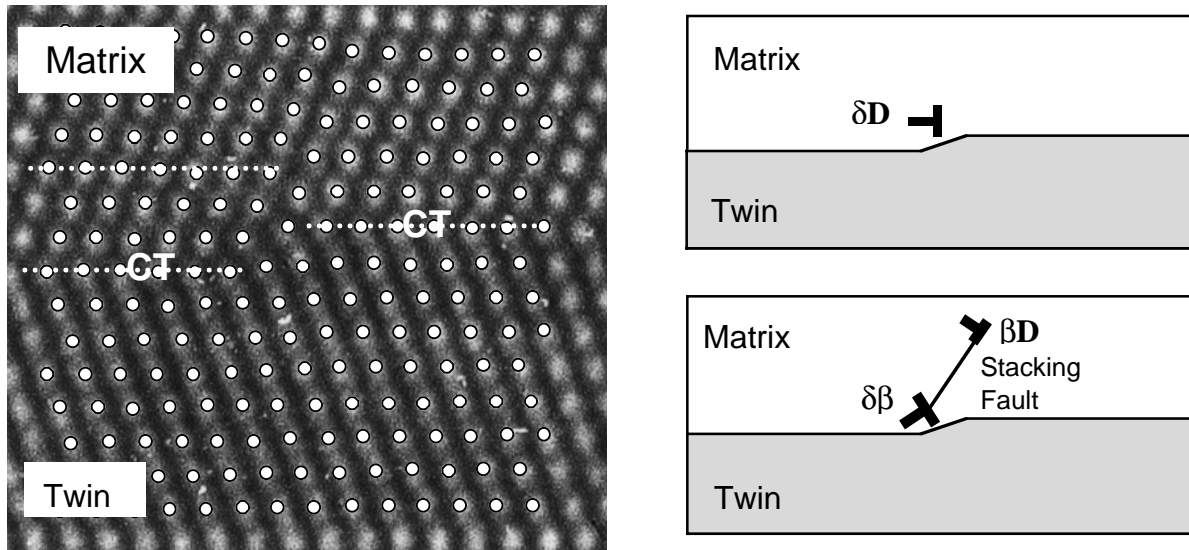Figure 2: Comparison of calculated structure for twin defect with experimental HRTEM observation. The circles are peak positions from an HRTEM image simulation.

3. Schematic illustrating dissociation of $\bar{1}]$ (δD) dislocation into a stair-rod dislocation ($\mathbf{b}$ $\bar{1}\,\bar{1}] = \delta\beta$) and a Shockley partial ($\mathbf{b}=\frac{1}{6}[\bar{2}\,\bar{1}\,\bar{1}] =$ slocation.

Extremely-Rapid Anisotropic Diffusion of Heteroepitaxial Islands on (100) Surfaces

J.C. Hamilton

Motivation:

Nucleation, growth, and diffusion of islands during initial film deposition largely determines structure of thin films. These processes are particularly difficult to control in heteroepitaxial thin films. Such films are of great technological importance, but their complex growth modes are not well understood. Previously we have discovered that cooperative dislocation mechanisms allow rapid diffusion of heteroepitaxial metal islands on close packed metal surfaces. However, heteroepitaxial islands will not diffuse on (100) planes by a dislocation mechanism because dislocation line energies are extremely large on these planes. Here we report a newly discovered mechanism for extremely rapid diffusion of heteroepitaxial islands on (100) surfaces. This mechanism accounts for the dramatic difference in heteroepitaxial film growth of Ag on Ni(100) compared to homoepitaxial growth of Ag on Ag(100).

Accomplishment:

Using molecular dynamics with embedded atom potentials for Ag and Ni, we have discovered a novel new diffusion mechanism for heteroepitaxial films on (100) surfaces. This mechanism applies to overlayer systems which reconstruct to form hexagonal overlayers. Examples include Ag on Ni(100) and Ag on Cu(100). In the case of Ag on Ni(100) there is a (8x2) reconstruction. The nature of this reconstruction can be seen in figure 1. The overlayer atoms form a close-packed island on the four-fold open substrate.

This reconstruction relieves the strain due to the large lattice mismatch between Ag and Ni. Along a single horizonal row of Ag atoms there are 7 Ag atoms for every 8 Ni atoms.

Since the Ag atoms lie in a variety of sites between hollow and bridge along this row, it takes very little energy to slide the row of Ag atoms along the horizontal direction. In the vertical direction, moving the overlayer requires moving some of the Ag atoms over the tops of Ni atoms which requires a great deal of energy. Consequently diffusion is very rapid along one direction of the reconstruction and very slow along the other direction.

This phenomena can be seen in figure 2 which plots the two center of mass coordinates of the island during a 2 nsec molecular dynamics run at 300K.

Significance:

There have been a number of experimental studies which have suggested rapid island diffusion for heteroepitaxial islands. These results have often been ignored or relegated to obscure publications perhaps because they have seemed inexplicable or improbable to the experimentalists. The discovery of rapid anisotropic diffusion for heteroepitaxial islands on (100) planes, indicates that rapid island diffusion may occur in many heteroepitaxial systems. Such rapid diffusion will have a major impact on our understanding of thin film growth, critical to semiconductor processing and other important technologies.

Publications: Rapid Anisotropic Diffusion Of Strained Overlayer Islands By Floating Phase Mechanism: Ag on Ni(100), in preparation for Physical Review Letters, J. C. Hamilton

Figures

start   finish
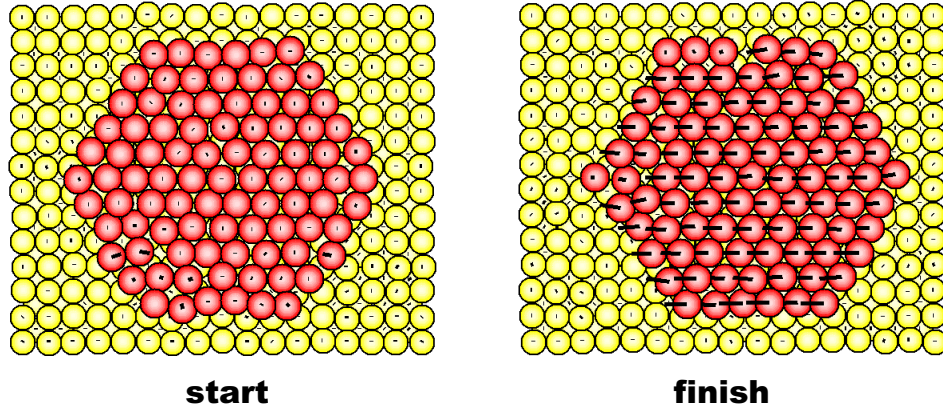
1) Starting configuration for 91 atom cluster of Ag on Ni(100) and configuration after 2nsec of molecular dynamics simulation of diffusion at 300K. Note that the Ag island exhibits a (8x2) reconstruction. The Ag atoms are in a hexagonal array, even though thesubstrate Ni has fourfold symmetry. The black lines show the displacements of the atoms from their initial positions. Note that cooperative gliding of the cluster in the horizontal direction occurs rapidly, but there is no diffusion in the vertical direction.
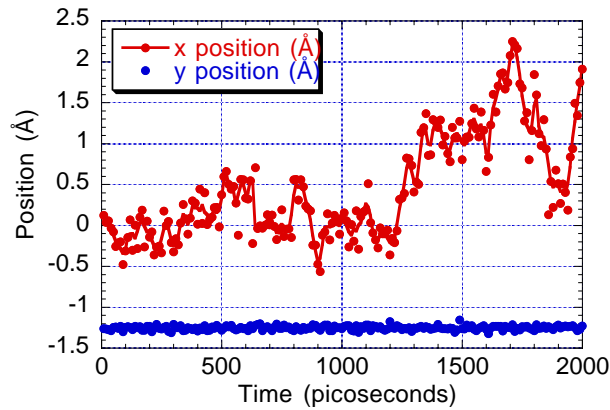
2) X and y coordinates of center of mass of 91 atom island as a function of time during 300K annealing for 2 nsec. There are a total of five collective hops in horizontal (x) direction during this run, but no diffusion occurs in the vertical (y) direction.

Short-Range Order and Phase Stability of Thin-Film Alloys

V. Ozolins, M. Asta, A. K. Schmid, N. C. Bartelt, and R. Q. Hwang

Motivation:

In heteroepitaxial growth a recently observed phenomenon is the formation of thin alloy layers that are localized near the film-substrate interface. This trend has proven to be remarkably general and it is commonly observed that two elements which are immiscible in the bulk alloy on the surface. Because interfacial structure is a dominant factor in the determination of thin-film properties, it is important to develop a detailed understanding of this alloying behavior. Such an understanding requires a thorough investigation of the thermodynamic properties of thin-film alloy systems.

Accomplishment:

We have succeeded in extending first-principles methods developed for bulk alloys in order to study the structure and phase stability of ordered and disordered thin-film alloys. Our approach has allowed electronic-structure and elastic-energy effects to be incorporated in the calculation of thin-film-alloy thermodynamic properties for the first time. Our calculations are being validated through direct comparison with atomic-resolution scanning-tunneling-microscopy (STM) images of alloy structures. Specifically, STM images are used to measure chemical short-range-order (SRO) parameters in thin-film-alloy solid-solutions equilibrated at well-characterized temperatures. This measured SRO data provides a basis for critically testing the predictions of the first-principles calculations. In Fig. 1 calculated and measured SRO parameters are compared for $Pd_{0.61}Au_{0.39}$ and $Cu_{0.67}Ag_{0.33}$ pseudomorphic monolayer alloys on Ru(0001). The agreement between experiment and theory is excellent; the stronger ordering in Pd-Au relative to Cu-Ag is reproduced by the calculations, as is the surprising result that the SRO parameters peak at third neighbor in Cu-Ag. Our calculations also are being used to investigate the phase stability of thin-film alloys. In Fig. 2 the results of simulated annealing calculations are shown for Pd_2Au and Cu_2Ag alloys on Ru(0001). In both cases disordered surface alloys undergo *ordering* transitions below room temperature. The predicted ground-state phases are shown in Fig. 2 and illustrate the variety of structures expected to form for different alloy systems.

Significance:

Our calculations are being used to determine the important thermodynamic factors affecting alloy phase stability at surfaces. The predictive computational framework being developed and validated in our work can be used to compute thin-film alloy phase diagrams. As in bulk alloys, these phase diagrams are useful for guiding the development of new thin-film materials with novel structures and properties.

Publications:

[1] B. Sadigh, M. Asta, V. Ozolins, A. K. Schmid, N. C. Bartelt, A. A. Quong and R. Q. Hwang, "Short-Range Order and Phase Stability of Surface Alloys: PdAu on Ru(0001)," submitted to Physical Review Letters.

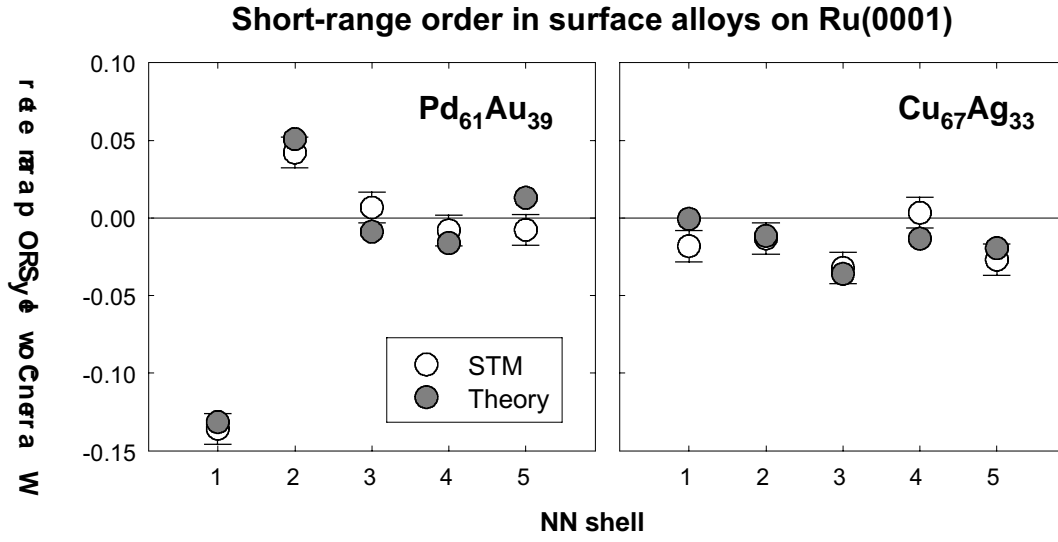**Short-range order in surface alloys on Ru(0001)**

Fig. 1: Experimentally-Measured (STM) vs. First-Principles-Calculated (Theory) SRO parameters for Pd-Au and Cu-Ag pseudomorphic alloys on Ru(0001).
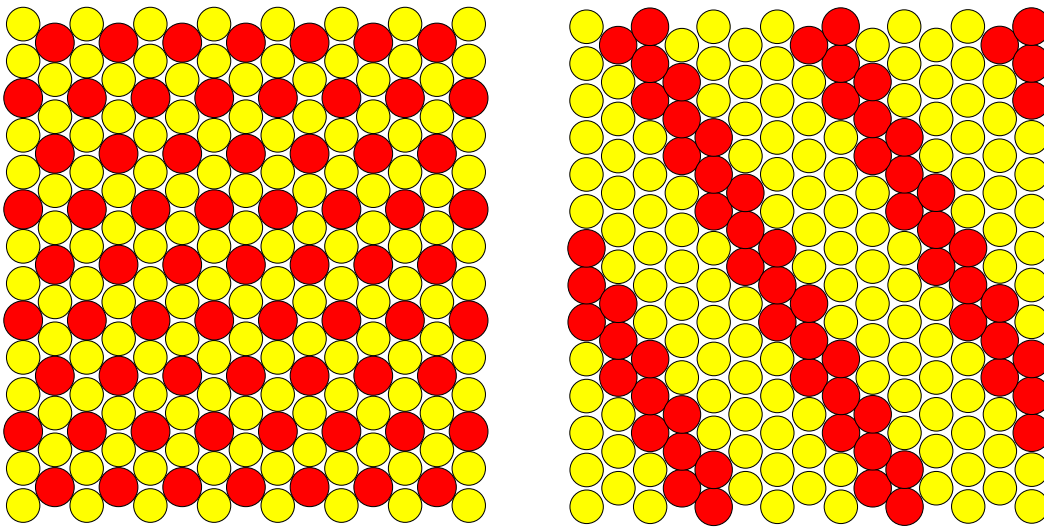

Fig. 2: Predicted ground-state structures for Pd_2Au (left) and Cu_2Ag (right) on Ru(0001).

Impact of Dislocation Networks on Interdiffusion
in Strained Epitaxial Films

A.K. Schmid and O. Schaff

Motivation:
Thin alloy films have many important applications. During film deposition, the kinetics and thermodynamics governing the structural evolution of the topmost atomic layer are key factors determining the properties of resulting films. While our understanding of the thermodynamics of thin film alloys is improving, phase transformation kinetics remain poorly understood. The challenge is to determine the atomic mechanisms relevant to phase transformations in surface layers. We have addressed the issue by using in-situ, atomic resolution microscopy to study interdiffusion kinetics in a suitable model system.

Accomplishment:
Due to misfit induced strain, networks of dislocations are a common property of epitaxial films. We have shown that the dislocations can be extremely mobile and play an important role in diffusive mass transport on surfaces [1]. Anticipating the strong impact mobile dislocation networks might have on the kinetics of alloying, we used the technique of annealing two-dimensional diffusion couples [2] to study a suitable model system. On top of a Ru(0001) substrate, we constructed diffusion couples consisting of monolayer regions of pure Pd, joined with monolayer regions of pure Au. The system was chosen because (i) Au/Ru(0001) features a well-ordered dislocation network, while the structure of Pd/Ru(0001) is free of dislocations, and (ii) Au and Pd are completely miscible on Ru(0001). The lightly annealed diffusion couple shown in figure 1 highlights the striking impact of dislocation dynamics on alloy formation kinetics in this prototypical system. The rate of interdiffusion strongly depends on the alignment of the linear Pd/Au interface with the underlying Ru lattice. Reflecting the threefold symmetry of the Ru substrate, three inert sections of the Pd/Au interface remain straight while three unstable sections of the interface appear jagged due to rapid interdiffusion. This novel phenomenon is caused by the strong link between mass transport and the structure of the dislocation network on the Au-rich side of the diffusion couple. Depending on interface orientation, dislocations either acts as barriers and drastically attenuate diffusion (figure 2a), or strongly promote intermixing by thermally activated dislocation climb across the interface (figure 2b).

Significance:
Surface alloy phase transformations involve phenomena one would not be able to predict by a simple comparison with bulk diffusion analogs. This work shows a new atomic mechanism through which phase transformations in thin film alloys are strongly linked to the structure and dynamics of dislocation networks.

Publications:

[1] A.K. Schmid, N.C. Bartelt, J.C. Hamilton, C.B. Carter, and R.Q. Hwang, "Brownian Motion of Dislocations in Thin Films," Phys. Rev. Lett. **78**, 3507 (1997).

[2] A.K. Schmid, J.C. Hamilton, N.C. Bartelt, and R.Q. Hwang, "Surface Alloy Formation by Interdiffusion across a Linear Interface," Phys. Rev. Lett. **77**, 2977 (1996).
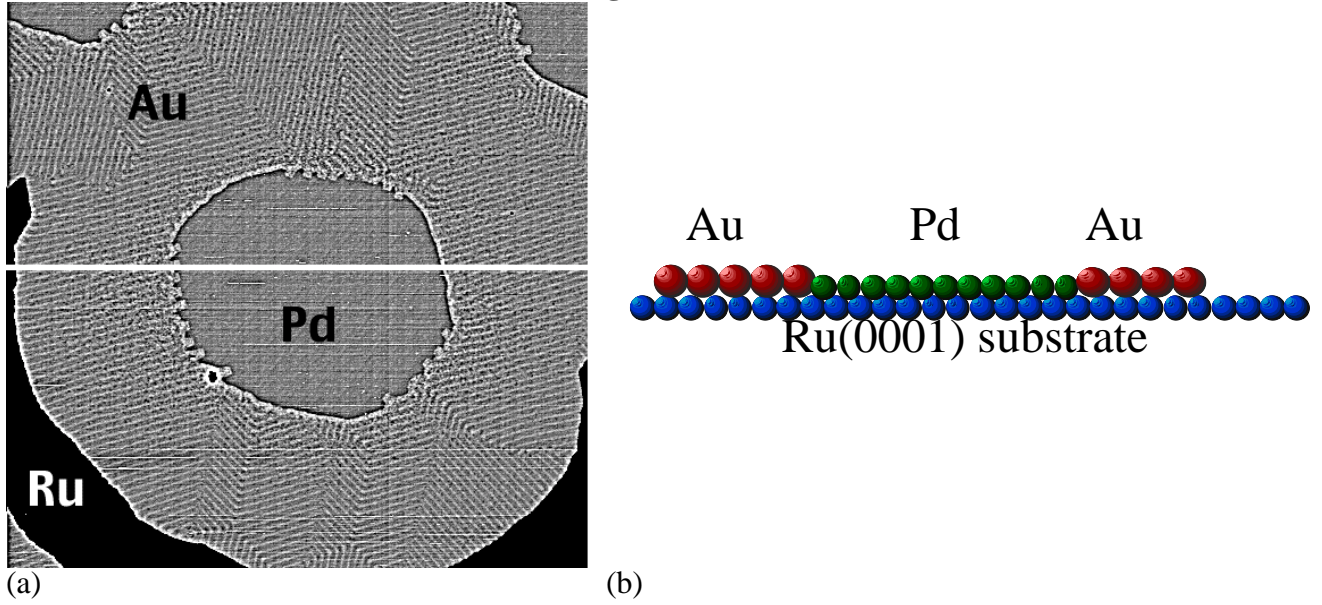
(a)   (b)

Figure 1: (a) STM image (300nm x 300nm) of a lightly annealed two-dimensional diffusion couple and (b) schematic crossection. The pattern of dark lines in the Au region in (a) is caused by the dislocation network. Three smooth sections of the Pd/Au interface reflect attenuated intermixing along these directions, while three jagged sections of the interface indicate rapid interdiffusion mediated by thermally activated dislocation climb.

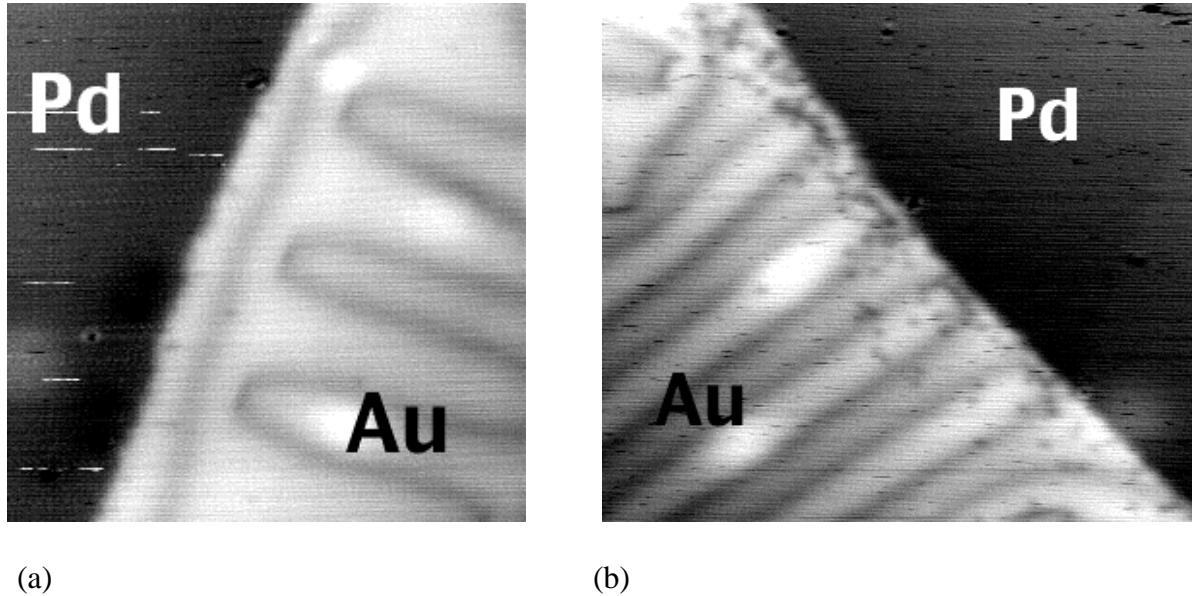(a)   (b)

Figure 2: Two sections of Pd/Au interface in detail. Dark lines in the Au region are Shockley partial dislocations. Along the section shown in (a) a stacking transition separates the pseudomorphic Pd region from the dislocation network in the Au region and attenuates intermixing. In (b) dislocations terminate directly at the Pd/Au interface and enhance intermixing.

Evolution of Dislocation Boundaries and Structures
Darcy Hughes and Andrew Godfrey

Motivation:
All processing of materials' shapes, whether by rolling, forging, or milling involves plastic deformation. The deformation microstructures that develop control the materials properties, functionality and range of applications. Identification of microstructural relationships which are invariant and/or scale during straining are important towards obtaining both fundamental understanding of microstructural evolution and to construct predictive physical models of deformation.

Accomplishment:
An invariant form for the observed microstructural evolution has been found experimentally. A simple model has been proposed to explore the observed scale invariance. Single crystals of aluminum were compressed and polycrystals of nickel were rolled to different strain levels. Transmission electron microscopy was performed on the deformed samples to measure the dislocation structure as a function of material and evolutionary state. Distributions of dislocation boundary spacings and the misorientation angles across them were obtained. A scaling hypothesis, based on the average spacing, was applied to the widely varying distributions. Remarkably all of the scaled distributions collapse into a single distribution as shown in Fig. 1. This distribution is very similar to that obtained previously for the scaled distributions of boundary misorientation angle. Those scaled distributions remain invariant under a wide range of materials and monotonic processing conditions.

To investigate the origins of the scaled distribution a simple model that considers the effect of introducing new boundaries into a preexisting structure has been made. In this model new boundaries are introduced in between older boundaries based on simple rules for their location in a prexisting array of boundaries. The average spacing between boundaries is thus decreased in this scheme. The results of this model are shown in Fig. 2 in which the evolution of the scaled boundary spacings in the model is very similar to that observed experimentally in Fig. 1.

Significance: The observed universality reveals that the microstructure is related to processing by simple rules that can be incorporated into predictive models. These rules are valid for a wide range of materials and process conditions and are needed to direct model selection. Predictive models are essential to lower production costs and energy consumption in high volume, energy intensive metal forming industries.

Publications:
D.A. Hughes, D.C. Chrzan, Q. Liu, N. Hansen, "Scaling of Misorientation Angle Distributions," Phys. Rev. Let., 81, 1998, p 4664. A. Godfrey and D.A. Hughes, "Scaling of Deformation Induced Dislocation Boundaries," in preparation. D. A. Hughes,
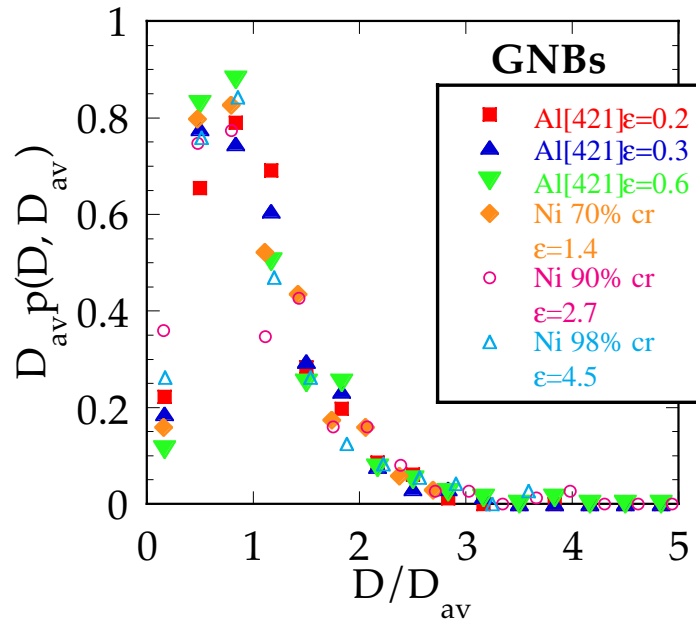
Fig. 1. Scaled probability distributions for GNB dislocation boundary spacings, D, for a wide strain range in aluminum and nickel. The average spacings, D_{av}, ranged form 4.5 to 0.13 µm.
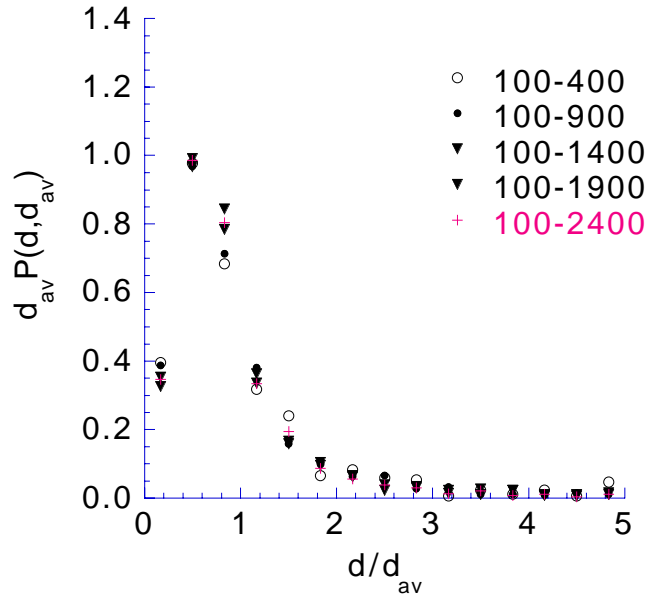

Fig. 2. Scaled spacing distributions obtained from a simple model that includes the effect of creating new dislocation boundaries in between the old ones. The observed shape of the caclulated distribution is similar to the experimental results. The number of new boundaries that has been added within the initial array of 100 boundaries is shown in the legend.

Discovery of Self-Limiting Growth During Formation of Metal/Ceramic Interfaces

D. A. Chen, M. C. Bartelt, R. Q. Hwang, and K. F. McCarty
Sandia National Laboratories, Livermore, CA 94550

Motivation:

    Metal/ceramic interfaces play critical roles in many technologies, including ceramic joining, metal/ceramic seals, chemical sensors, catalysts, and microdevices. Optimization of performance and development of new technologies can be greatly aided through basic understanding how metal/ceramic interfaces form, evolve, and affect ultimate system performance. To this end, we have studied how a metal (copper) grows on a model ceramic (rutile) under well-characterized conditions.

Accomplishment:

    The rutile (110) surface consisted of atomically flat terraces about 100 Å in width separated by unit-cell-high steps. The nucleation of copper on rutile (TiO_2) was studied using scanning tunneling microscopy (STM) under ultrahigh vacuum conditions. The resulting copper islands nucleated preferentially at step edges and grew in three dimensions (3D). That is, rather than growing laterally and covering the substrate (i.e., 2D growth), the Cu islands grow up, forming islands with high aspect ratios (see Figure). Computer simulations showed that the observed 3D islands can only form if there is an "upflow" of deposited copper atoms from the rutile surface onto the Cu islands. A striking behavior was discovered in the dependence of island size and density with increasing Cu dose -- namely, the Cu islands grow to a temperature-dependent size and then essentially stop growing. Addition Cu dosing produces new islands (i.e., additional nucleation), but not larger particles. We believe that this *self-limiting* behavior results from the island-size dependence of the Cu "upflow" from the substrate onto the islands. This behavior is in marked contrast to conventional film growth (e.g., formation of metal/metal interfaces), for which increased deposition results in island growth and no addition nucleation.

Significance:

    Scientifically, our findings establish a new mechanism of interface formation that occurs because of the greatly differing properties of the metal and ceramic. Because the metal interacts weakly with the ionic substrate and prefers to bond to itself, the deposited copper diffuses from the substrate onto the Cu islands, giving 3D growth. But the "upflow" process stops when the metal particle reaches a critical size, producing a unique self-limiting growth. Technologically, our discovery has impact in two broad areas. First, self-limiting growth may be the underlying mechanism controlling grain structure in metal films on ceramics. That is, the process limits the island size, which in turn sets the length scale of grains in the resulting film. Second, our discovery offers a way to make metal particles with a narrow size distribution. The particle size can be altered simply by changing the deposition temperature. Narrow sizes are desired for technologies such as quantum-dot electronics, chemical sensors, and catalysts.
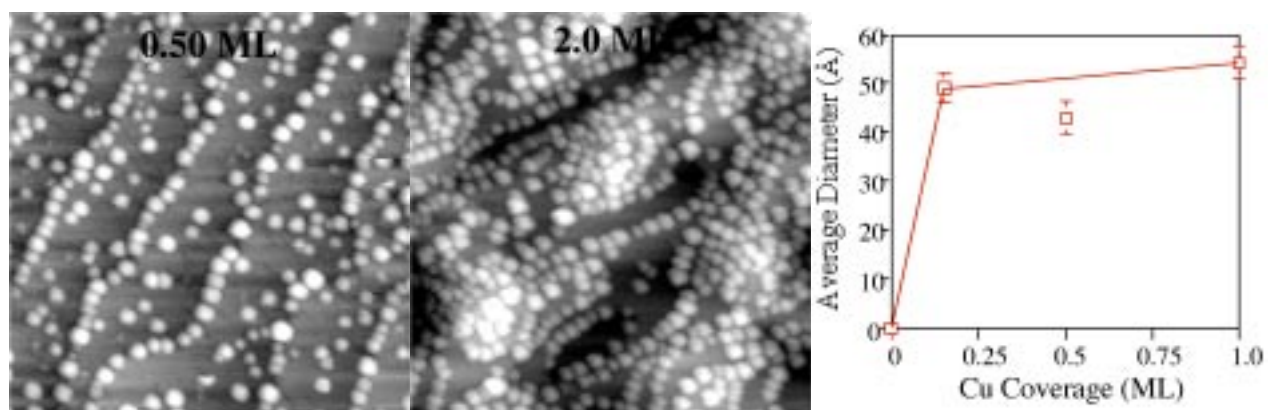
Figure caption. STM images (1000 x 1000 Å) of a rutile (110) surface dosed with 0.5 (left) and 2.0 (middle) monolayers of Cu. With increased dose, the Cu particles hardly increase in sizes but the number of particles increases greatly. The plot (right) shows the saturation of island diameter at low Cu dose.

Atomistic Simulations of Liquid-Alloy Thermodynamic and Kinetic Properties

Jeff Hoyt and Mark Asta, Sandia National Laboratories, Livermore, CA
Didier de Fontaine, University of California at Berkeley
Duane Johnson, University of Illinois

Motivation:

The structural, thermodynamic and atom-transport (eg., diffusion, viscosity) properties of liquid metal alloys play critical roles in many technologically-relevant materials processing procedures. Additionally, these properties govern the quench-rate required to access the glass transition. In spite of the significant practical importance of liquid-alloy properties in general, little experimental data is available for most binary and practically all multicomponent systems. We are developing and validating first-principles and semiempirical atomic-scale, computer-simulation techniques to calculate kinetic and thermodynamic properties of multicomponent liquid metal alloys.

Accomplishment:

The structural, thermodynamic and kinetic properties of elemental late-transition-metal liquids have been calculated using classical Molecular-Dynamics (MD) and Monte-Carlo (MC) simulations based upon Embedded-Atom-Method (EAM) semiempirical atomic potentials [1]. This work includes the first calculation of solid-liquid interface velocities as a function of undercooling and crystallographic orientation (Fig. 1). We find that the EAM framework provides accurate results for the properties of late-transition-metal alloys characterized by nearly ideal solution thermodynamics. However, recent simulations for Ni-Al [2] point to limitations of the EAM for concentrated alloys possessing strong chemical short-range-order (SRO). First-principles simulations are underway to understand the electronic origins (charge-transfer and hybridization) of the strong chemical SRO in Ni-Al. These results will be used to guide the development of more accurate potential models for transition-metal liquid alloys.

Significance:

Atomic-scale computer simulations are being used to calculate kinetic and thermodynamic parameters required in phase-field models of microstructural evolution during solidification. These simulations will allow, for the first time, solidification-microstructure models to be applied to specific alloy systems (such as Cu-Ni and Cu-Ag) used in brazing applications. Simulations of kinetic and thermodynamic properties relevant for solidification and glass formation (e.g., solid-liquid free energies and interface velocities) require numbers of atoms well beyond current capabilities for *ab-initio* techniques. The modeling of liquid alloy properties therefore requires the development of reliable interatomic potentials guided by an understanding of the important electronic-structure details which affect chemical and topological short-range order in the liquid phase.

Publications:

[1] J. J. Hoyt, B. Sadigh and M. Asta, "Kinetic Phase Field Parameters for the Cu-Ni System Derived from Atomistic Computations," submitted to Acta Materialia.
[2] M. Asta, D. Morgan, J. J. Hoyt, B. Sadigh, J. D. Althoff, D. de Fontaine and S. M. Foiles, "Embedded-Atom-Method Study of Structural, Thermodynamic and Atom-Transport Properties of Liquid Ni-Al Alloys," submitted to Physical Review B.
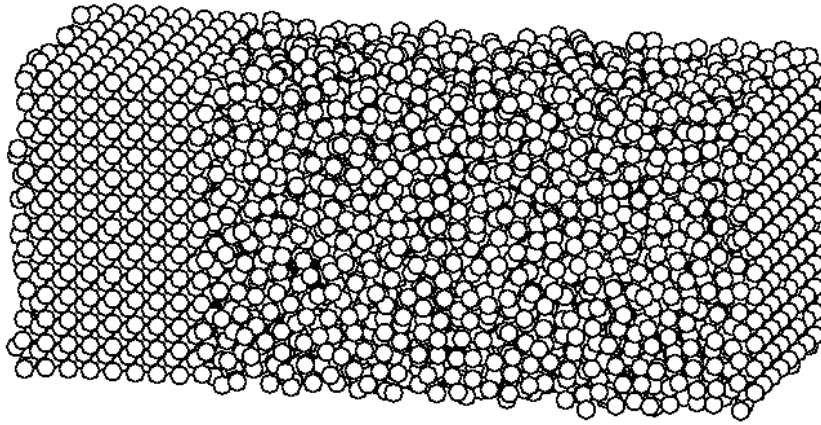
(a)
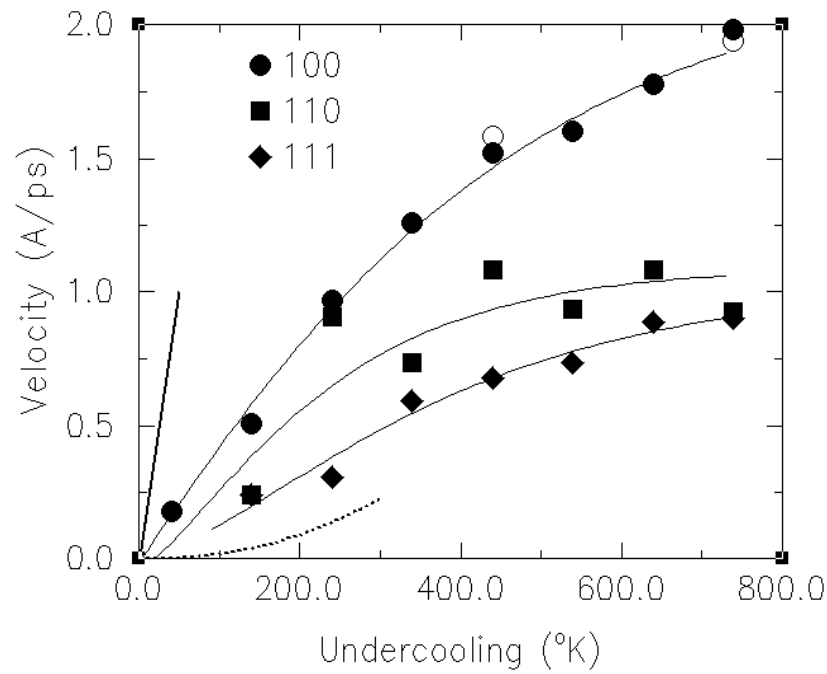
(b)

Figure 1. (a) Initial simulation for the computation of the solid-liquid interface velocity in Ni. Solid portion on the left of the figure is oriented with [100] perpendicular to the growth direction. (b) Planar solid-liquid interface velocity as a function of undercooling for the 100,110 and 111 directions in Ni. The solid line is the theoretical upper limit and the dashed line is experimental results for dendrites.

Thermal Vibrations of Misfit Dislocations
In Thin Metal Films

N.C. Bartelt, J. de la Figuera and R.Q. Hwang

Motivation:

The energy required to bend a dislocation is a fundamental quantity which governs many important materials properties. Dislocation stiffness determines, for example, the value of the applied stress necessary to drive dislocations through a network of pinning sites, and thus is important in understanding the strength of materials. In our work we have coupled experiment and theory to understand what determines the bending stiffness of misfit dislocations in thin metal films. Models of dislocations usually make many untested simplifying assumptions. Our work directly probes the validity of these assumptions.

Accomplishment:

Our experimental approach is to use atomic resolution scanning tunneling microscopy to measure the amplitude of thermally generated vibrations in dislocations in thin metal films. Figure 1 shows an STM image of a 500Å long misfit dislocation in a Cu monolayer on the close packed surface of Ru. The pairs of bright stripes in the image represents a single row of atoms which has been inserted into the triangular lattice of Cu atoms. (This simple misfit dislocation appears as a pair of features in the STM image because it has decomposed into a pair of Shockley partial dislocations.) At zero temperature, this dislocation would be perfectly straight because of the energy cost of bending. As seen from the figure, however, we observe that thermal fluctuations cause the dislocations to vibrate. By assuming equipartition of thermal energy amongst vibrational modes we can determine the dislocations bending stiffness from the measured amplitude of the vibrations. To interpret the measured stiffness, we use the two-dimensional Frenkel-Kontorova model, combined with first-principles calculations of the interatomic potential between the Cu atoms. An example of the structure of a bent dislocation in this model is shown in Figure 2. By computing the energy of such structures, we have found the general relationship between the elastic constants controlling the energy of elastic distortions of the 2-D Cu layer and the dislocation stiffness. We find that while the energy to create the dislocations is determined primarily by the bulk modulus of the 2-D film, the bending stiffness is determined by the shear modulus. Our first principles calculations of the shear modulus show that standard simple spring models of the Cu—Cu interatomic potential are inadequate. The final bending stiffness we compute from first principles is within a factor of two of the experimentally observed value, suggesting that the classical Frenkel-Kontorova model provides a reasonable account of the energetics of misfit dislocations (as long as one does not assume simple springs between atoms). Our Frenkel-Kontorova model also predicts a negligible Peierls barrier for the dislocation motion, consistent with our experimental observations that the vibrations are readily thermally activated at room temperature.

Significance:

The bending stiffness of a dislocation has been directly measured for the first time: we find that measured stiffness can be well described by the simple 2-D Frenkel Kontorova model, although the final result requires an accurate knowledge of the nature of interactions between metal atoms.

Publications:

"Thermal Vibrations of Misfit Dislocations in Thin Metal Films," by J. de la Figuera, N.C. Bartelt and R.Q. Hwang, in preparation.

Figures
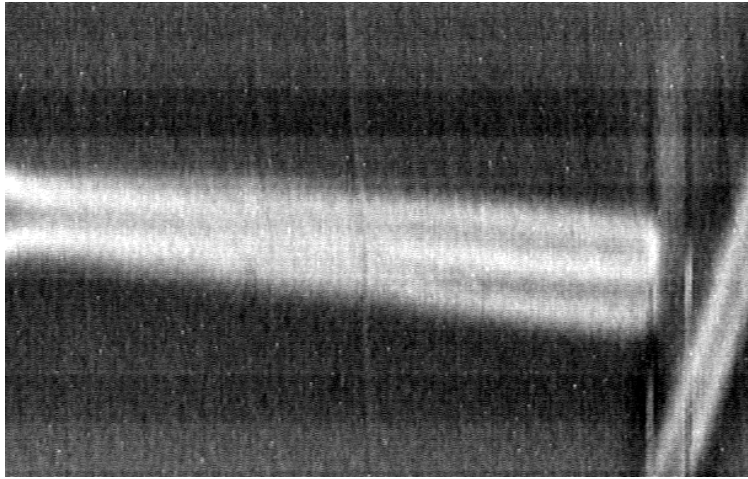
2) A 600ÅX300Å STM image of a fluctuating misfit dislocation in a single monolayer film of Cu on Ru(0001) at room temperature. The frequency of the vibrations is much faster than the image acquisition time, so the dislocations appears blurred. The dislocation is most distinct at the limits of its motion, when it is traveling most slowly.
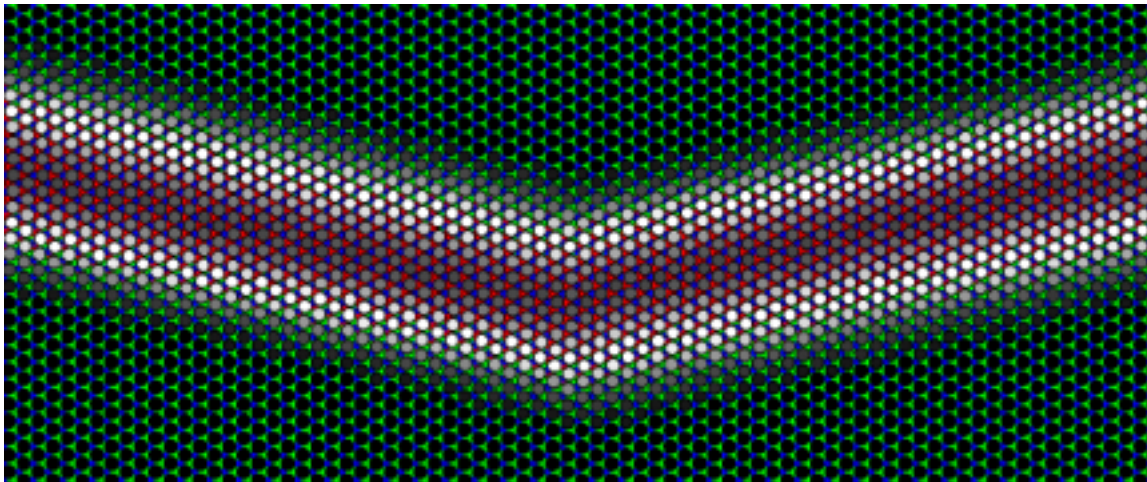
2) A Frenkel-Kontrova atomic model of a bent misfit dislocation. The interactions between atoms was taken from first principles electronic structure calculations. The resulting structure of the dislocation matches experimental observations. In the green regions of the figure, the Cu atoms (circles) are sitting in hcp sites on the Ru substrate; in the red regions the Cu atoms are in fcc sites. The brightness of the Cu atoms represents their height above the substrate. The energy cost of such a bent structure was used to compute the stiffness of the dislocation.